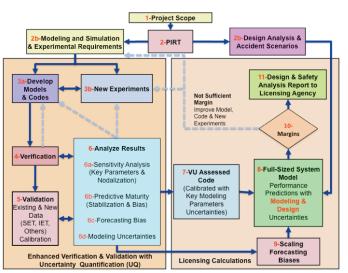
## Improved Methodology for Estimation, Uncertainty, and Validation for Licensing of Evolving Nuclear Reactors

Cetin Unal, D-DO; Brian J. Williams, CCS-6; Christopher J. Stull, INST-OFF; David M. Higdon, CCS-6 A methodology that can potentially be used to address new challenges in the design and licensing of evolving nuclear technology has been developed [1]. The methodology is generic and can be used as a certification/licensing framework in other technology areas including defense, energy and environment, and basic and applied research and science projects. The main components of the proposed methodology are verification, validation, calibration, and uncertainty quantification—steps similar to the components of the traditional US Nuclear Regulatory Commission (NRC) licensing approach with the exception of the calibration step. An enhanced calibration concept is introduced here, and is accomplished through data assimilation. The new methodology suggests a formalism to quantify an adequate level of validation (predictive maturity [2]) with respect to existing data so that additional experimental testing can be minimized, reducing costs by demonstrating that this testing will not enhance the quality of the predictive tools.

Fig. 1. Overview of the improved best estimate plus uncertainty methodology.



pplication of the advanced validation methodology of Fig. 1—involving verification, validation, calibration, and uncertainty quantification—to the nuclear fuel performance codes FRAPCON and LIFEIV was performed for the Nuclear Energy Advanced Modeling and Simulation (NEAMS) program. FRAPCON is used to predict oxide fuel behavior in light water reactors (LWR). LIFEIV was developed in the 1980s to predict oxide fuel behavior in fast reactors. We utilize a

screening methodology to narrow down the selected parameters for sensitivity and calibration analyses. We deployed the screening methods to both codes and discussed results. The number of modeling parameters selected was 61 for FRAPCON and 69 for LIFEIV. Screening resulted in only 24 parameters of importance for FRAPCON, while the LIFEIV analysis reduced important modeling parameters to 34.

LIFEIV sensitivity studies indicated that the fuel thermal conductivity and gas release models were most influential in terms of explaining overall output variability after calibration to available pin data, and are therefore targets for additional calibration to further constrain their parameters. For example, Fig. 2 shows the change in average fission gas release induced by calibrated marginal variation in each of 18 LIFEIV calibration parameters, along with a measure of variability in fission gas release induced by these calibrated single-parameter effects. Residual (post-calibration) uncertainties in parameters TC2 (fuel thermal conductivity) and FGPM1 (fission gas release) have the most pronounced effects on fission gas release, and are thus candidates for further uncertainty reduction.

The gap thermal conductance and crack elasticity models had a less pronounced effect on overall output variability. We combined these results with the results of the screening study to recommend a ranking of models that can be considered for further improvements. Our model ranking is as follows:

- fuel creep;
- · fuel conductivity;
- fission gas transport/release;
- · crack/boundary; and
- fuel gap conductivity.

We think a major review of the fuel creep model and uncertainties associated with its parameters is needed urgently. Means of calibrated parameter distributions were compared with nominal LIFEIV values,

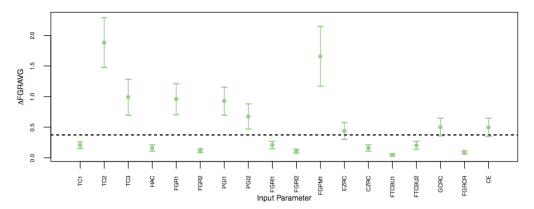


Fig. 2. Post-calibration sensitivity analysis of 18 LIFEIV calibration parameters (x-axis) on average fission gas release (y-axis).

indicating that changes of up to  $\pm 10\%$  can be observed. This effort will continue with assessment of calibrated model predictions against additional independent validation pin data.

FRAPCON sensitivity results primarily agreed with results obtained from LIFEIV and indicated that the fuel thermal conduction and fission gas release models are two key modeling areas on which to concentrate for further reduction of uncertainty. The following particular parameters were found to be important contributors.

## Thermal Conduction

- phonon term in thermal conduction model;
- porosity correction to thermal conduction accounting for radiation effects; and
- overall fuel thermal conductivity.

## Fission Gas Release

- multiplier in grain boundary accumulation model;
- saturation area density gas multiplier;
- burn-up enhancement factor applied to diffusion constant; and
- diffusion constant multiplier.
- Design Parameters and Indirect Modeling Parameters
  - pod surface heat flux at elevation z on the rod axis; and
  - as-fabricated fuel-cladding gap size.

The four fission gas release calibration parameters were further investigated with a larger set of data. It was found that the adjustment to activation energy was the most sensitive parameter in predicting gas release fraction if other modeling parameters (especially the fuel conduction model) were not considered.

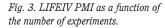
"When is a prediction from a numerical model good enough?" All too often, the answer to this question relies on expert opinion: a qualitative and subjective answer on which to rely, given the quantitative nature of verification, validation, and uncertainty quantification. To address this concern, researchers at LANL have been investigating a metric referred to as the Predictive Maturity Index (PMI). The PMI offers a succinct and quantitative mechanism by which to track year-to-year improvements of a numerical model, while also providing a description of particular areas that need improvement. The PMI currently takes four attributes into account:

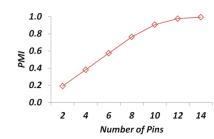
- coverage of the design space over which the models are applied;
- discrepancy between the model predictions and the experimental data:
- complexity of the model, relative to the state-of-the-art models; and
- robustness of the models to lack of knowledge on the part of the analyst(s).

An example of this framework applied to the LIFEIV calibration study is given in Fig. 3 where it is seen that the addition of pins to the suite of available experimental data results in a corresponding increase in the value of the PMI.

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<sup>[1]</sup> Unal, C., et al., Nucl Eng Des 241, 1813 (2011).

<sup>[2]</sup> Hemez, F. et al., Comput Struct 88, 497 (2010).